# PipPhos and MorfPhos

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# CIF-file generated for C56H40N2O4P2                          CP838
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# 0. AUDIT DETAILS

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 SHELXL97-2 & Manual Editing
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_audit_update_record
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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
   Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
     Crystal Structure Center,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;
_publ_contact_author_email           A.Meetsma@fwn.rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal                      ?
# Publication choise FI FM FO CI CM CO
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2004-08-06  13:54:54

 Consider this CIF submission for deposition of the (first)
 X-ray structure of a manuscript to be submitted to : JOC
  (Our Compound_Identification_Code : CP838)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

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_journal_date_from_coeditor          ?
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_journal_date_printers_first         ?
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_journal_date_proofs_out             ?
_journal_date_proofs_in              ?

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; ?
;

_journal_techeditor_code             ?
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_journal_issue                       ?
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_journal_suppl_publ_pages            ?


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# 3. TITLE AND AUTHOR LIST

_publ_section_title
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;
_publ_section_title_footnote
;
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;

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address

   'Meetsma, Auke'
;
 ? # author related footnote
;
;
     Crystal Structure Center,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;

#==============================================================================
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# 4. TEXT

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;
_publ_section_abstract
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;

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;
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;
_publ_section_exptl_refinement
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;

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 Beurskens, P.T., Beurskens, G., Gelder, R. de   Garc\'ia-Granda, S.
  Gould, R.O.  Isra\"el, & Smits, J.M.M. (1999).
  The DIRDIF99 program system, Technical Report of the Crystallography
  Laboratory, University of Nijmegen, The Netherlands.

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  Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

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   Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
   (Present distributor Kluwer Academic Publishers, Dordrecht).

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   Edited by A.J.C Wilson, Kluwer Academic Publishers,
   Dordrecht, The Netherlands.

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   Groningen University, The Netherlands. (unpublished).

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   Refinement. University of G\"ottingen, Germany, 1997.

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   University of G\"ottingen, Germany, 2001

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```

```
 Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

 Spek, A.L. (1990). Acta Cryst. A46, C-34.

 Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.
;


_publ_section_figure_captions
;
     Fig. 1. Chemical structural diagram (scheme 1) of the title compound

     Fig. 2. Perspective PLUTO drawing of the molecule illustrating the
             configuration and the adopted numbering scheme.

     Fig. 3. Molecular packing viewed down unit cell axes.

     Fig. 4. Perspective ORTEP drawing of the title compound.
             Displacement ellipsoids for non-H are represented at the 50%
             probability level.
             The H-atoms are drawn with an arbitrary radius.
;

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# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common                 ?
_chemical_melting_point               ?
_chemical_formula_moiety
'C28 H20 N O2 P'
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
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_chemical_formula_sum
'C28 H20 N O2 P'
_chemical_formula_iupac               ?
_chemical_formula_weight                 433.44
_chemical_compound_source            'see text'

loop_
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_atom_type_scat_dispersion_imag
_atom_type_scat_source
 P   P    0.1023    0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 O   O    0.0106    0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 N   N    0.0061    0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H    0.0000    0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#==============================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting                Orthorhombic
_symmetry_space_group_name_Hall       'P 2ac 2ab'
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_symmetry_space_group_name_H-M       'P 21 21 21'
_symmetry_Int_Tables_number                19

loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 1/2-x,-y,1/2+z
 1/2+x,1/2-y,-z
 -x,1/2+y,1/2-z

_cell_length_a                         10.1891(4)
_cell_length_b                         15.7633(7)
_cell_length_c                         26.655(1)
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_cell_volume                          4281.2(3)
_cell_formula_units_Z                    8

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      9870
_cell_measurement_theta_min        2.38
_cell_measurement_theta_max       29.54
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   9870 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'block'
_exptl_crystal_colour            'colorless'
_exptl_crystal_size_max           0.48
_exptl_crystal_size_mid           0.41
_exptl_crystal_size_min           0.22
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.345
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1808
_exptl_absorpt_coefficient_mu     0.155
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2000))'
_exptl_absorpt_correction_T_min   0.879
_exptl_absorpt_correction_T_max   0.966


#===============================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature            100(1)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                'MoK\a'
_diffrn_radiation_source              'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
```

```
;
_diffrn_measurement_method           'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean     '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number             ?
_diffrn_standards_interval_count     ?
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loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              39190
_diffrn_reflns_av_R_equivalents    0.0438
_diffrn_reflns_av_sigmaI/netI      0.0438
_diffrn_reflns_limit_h_min         -13
_diffrn_reflns_limit_h_max         13
_diffrn_reflns_limit_k_min         -21
_diffrn_reflns_limit_k_max         18
_diffrn_reflns_limit_l_min         -35
_diffrn_reflns_limit_l_max         35
_diffrn_reflns_theta_min           2.38
_diffrn_reflns_theta_max           28.28
_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.999

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
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_reflns_number_gt                  9568
_reflns_threshold_expression       I>2\s(I)


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_computing_data_reduction           'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
 DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 PLATON (Spek, 1994)
;
_computing_publication_material      'PLATON (Spek, 1990)'

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# 8. REFINEMENT DATA
```

```
_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0633P)^2^+0.0P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     refall
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details
;
   Flack, H.D. & Bernardinelli, G. (1999, 2000)
;
_chemical_absolute_configuration  ad

_refine_ls_abs_structure_Flack    -0.01(5)
_refine_ls_number_reflns          10565
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_refine_ls_number_restraints      0
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_refine_ls_R_factor_gt            0.0385
_refine_ls_wR_factor_ref          0.0971
_refine_ls_wR_factor_gt           0.0957
_refine_ls_goodness_of_fit_ref    0.993
_refine_ls_restrained_S_all       0.993
_refine_ls_shift/su_max           0.036
_refine_ls_shift/su_mean          0.001

_refine_diff_density_max          0.681
_refine_diff_density_min         -0.250
_refine_diff_density_rms          0.051


_vrn_publ_code_squeezed_elec        0.0
_vrn_publ_code_void_volume          0.0
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_vrn_publ_code_meas_time_hour       8.0

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_atom_site_fract_z
_atom_site_occupancy
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_atom_site_calc_flag
_atom_site_refinement_flags
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O11 O Uani 0.36278(12) 0.69226(8) -0.00142(4) 1.000 0.0212(3) . .
O12 O Uani 0.37094(12) 0.57539(8) 0.06187(4) 1.000 0.0210(3) . .
N1 N Uani 0.55001(14) 0.57291(11) -0.00012(6) 1.000 0.0262(4) . .
C11 C Uani 0.40690(17) 0.74739(11) 0.03617(6) 1.000 0.0202(5) . .
C12 C Uani 0.50990(18) 0.80279(13) 0.02304(7) 1.000 0.0265(5) . .
C13 C Uani 0.55768(19) 0.85756(13) 0.05817(8) 1.000 0.0279(6) . .
C14 C Uani 0.50813(16) 0.85776(11) 0.10785(7) 1.000 0.0220(5) . .
C15 C Uani 0.56359(17) 0.91052(12) 0.14523(7) 1.000 0.0251(5) . .
C16 C Uani 0.52016(18) 0.90760(12) 0.19362(7) 1.000 0.0263(5) . .
C17 C Uani 0.41926(18) 0.85125(12) 0.20688(7) 1.000 0.0234(5) . .
C18 C Uani 0.36148(16) 0.80000(11) 0.17154(6) 1.000 0.0195(4) . .
C19 C Uani 0.40302(15) 0.80214(11) 0.12073(6) 1.000 0.0179(4) . .
C110 C Uani 0.34793(16) 0.74790(10) 0.08273(6) 1.000 0.0172(4) . .
C111 C Uani 0.23674(15) 0.68893(11) 0.09284(6) 1.000 0.0167(4) . .
C112 C Uani 0.11117(16) 0.71635(11) 0.11181(6) 1.000 0.0188(4) . .
C113 C Uani 0.07981(17) 0.80289(13) 0.12050(7) 1.000 0.0231(5) . .
C114 C Uani -0.04202(19) 0.82573(14) 0.13798(7) 1.000 0.0294(6) . .
C115 C Uani -0.13921(19) 0.76451(15) 0.14712(8) 1.000 0.0318(6) . .
C116 C Uani -0.11334(17) 0.68091(14) 0.13843(7) 1.000 0.0275(5) . .
C117 C Uani 0.01141(16) 0.65443(12) 0.12030(6) 1.000 0.0222(5) . .
C118 C Uani 0.03614(17) 0.56804(12) 0.11009(7) 1.000 0.0239(5) . .
C119 C Uani 0.15332(18) 0.54327(11) 0.08986(7) 1.000 0.0229(5) . .
C120 C Uani 0.25171(16) 0.60429(11) 0.08140(6) 1.000 0.0194(4) . .
C121 C Uani 0.61408(17) 0.52246(11) -0.03623(6) 1.000 0.0209(5) . .
C122 C Uani 0.56408(19) 0.48594(13) -0.07949(7) 1.000 0.0260(5) . .
C123 C Uani 0.6496(2) 0.43965(13) -0.11006(8) 1.000 0.0318(6) . .
C124 C Uani 0.7802(2) 0.42932(15) -0.09736(9) 1.000 0.0374(7) . .
C125 C Uani 0.82823(19) 0.46428(15) -0.05345(9) 1.000 0.0365(7) . .
C126 C Uani 0.74523(17) 0.51102(12) -0.02275(7) 1.000 0.0243(5) . .
C127 C Uani 0.77032(18) 0.55223(15) 0.02726(8) 1.000 0.0306(6) . .
C128 C Uani 0.6510(2) 0.60755(18) 0.03505(10) 1.000 0.0431(7) . .


H12 H Uiso 0.55014 0.80098 -0.01050 1.00(3) 0.0140(18) . .
H13 H Uiso 0.62654 0.90024 0.05292 1.00(4) 0.039(2) . .
H15 H Uiso 0.63260 0.94284 0.13676 1.00(4) 0.033(2) . .
H16 H Uiso 0.56424 0.94083 0.21660 1.00(5) 0.039(2) . .
H17 H Uiso 0.38926 0.85005 0.24037 1.00(4) 0.022(2) . .
H18 H Uiso 0.29240 0.76515 0.17955 1.00(4) 0.026(2) . .
H113 H Uiso 0.14415 0.84609 0.11364 1.00(4) 0.020(2) . .
H114 H Uiso -0.05882 0.88265 0.14198 1.00(4) 0.032(2) . .
H115 H Uiso -0.22427 0.78313 0.15986 1.00(4) 0.034(2) . .
H116 H Uiso -0.18395 0.64078 0.14463 1.00(4) 0.025(2) . .
H118 H Uiso -0.03374 0.53059 0.11654 1.00(4) 0.023(2) . .
H119 H Uiso 0.17061 0.48601 0.08329 1.00(4) 0.026(2) . .
H122 H Uiso 0.47837 0.49360 -0.09038 1.00(5) 0.046(3) . .
H123 H Uiso 0.62071 0.41797 -0.14226 1.00(4) 0.041(2) . .
H124 H Uiso 0.83310 0.40115 -0.11880 1.00(4) 0.035(2) . .
H125 H Uiso 0.92266 0.45545 -0.04276 1.00(4) 0.043(3) . .
H127 H Uiso 0.84855 0.58202 0.02911 1.00(4) 0.034(2) . .
H127' H Uiso 0.77866 0.50501 0.05537 1.00(4) 0.047(3) . .
H128 H Uiso 0.61271 0.61084 0.06685 1.00(5) 0.057(3) . .
H128' H Uiso 0.67410 0.67463 0.02627 1.00(8) 0.125(4) . .


P2 P Uani 0.25039(4) 0.30923(3) 0.21381(2) 1.000 0.0203(1) . .
O21 O Uani 0.28446(11) 0.20980(8) 0.19797(5) 1.000 0.0220(3) . .
O22 O Uani 0.38342(11) 0.35507(8) 0.19047(4) 1.000 0.0211(3) . .
N2 N Uani 0.13321(13) 0.32236(10) 0.17086(5) 1.000 0.0227(4) . .
C21 C Uani 0.40186(16) 0.17833(11) 0.21752(6) 1.000 0.0200(4) . .
C22 C Uani 0.39503(18) 0.12650(12) 0.26069(7) 1.000 0.0245(5) . .
C23 C Uani 0.50786(18) 0.09356(12) 0.28011(7) 1.000 0.0240(5) . .
```

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C24 C Uani 0.63168(17) 0.11270(11) 0.25844(6) 1.000 0.0201(5) . .
C25 C Uani 0.75037(19) 0.08177(12) 0.27943(7) 1.000 0.0246(5) . .
C26 C Uani 0.86881(19) 0.10609(12) 0.26120(7) 1.000 0.0269(5) . .
C27 C Uani 0.87541(17) 0.16367(12) 0.22066(7) 1.000 0.0249(5) . .
C28 C Uani 0.76297(16) 0.19270(11) 0.19847(6) 1.000 0.0201(5) . .
C29 C Uani 0.63738(16) 0.16730(10) 0.21553(6) 1.000 0.0177(4) . .
C210 C Uani 0.51751(15) 0.19741(11) 0.19349(6) 1.000 0.0169(4) . .
C211 C Uani 0.51563(15) 0.25123(11) 0.14731(6) 1.000 0.0172(4) . .
C212 C Uani 0.58039(15) 0.22629(12) 0.10184(6) 1.000 0.0194(5) . .
C213 C Uani 0.63787(17) 0.14493(12) 0.09585(7) 1.000 0.0245(5) . .
C214 C Uani 0.7055(2) 0.12475(16) 0.05276(8) 1.000 0.0333(6) . .
C215 C Uani 0.7165(2) 0.18463(18) 0.01342(7) 1.000 0.0381(7) . .
C216 C Uani 0.6561(2) 0.26159(16) 0.01686(8) 1.000 0.0336(6) . .
C217 C Uani 0.58520(17) 0.28414(13) 0.06049(7) 1.000 0.0238(5) . .
C218 C Uani 0.52039(17) 0.36351(13) 0.06459(7) 1.000 0.0260(5) . .
C219 C Uani 0.45369(16) 0.38460(12) 0.10696(7) 1.000 0.0235(5) . .
C220 C Uani 0.44993(15) 0.32776(11) 0.14768(6) 1.000 0.0192(5) . .
C221 C Uani 0.01361(15) 0.36512(11) 0.18015(7) 1.000 0.0207(5) . .
C222 C Uani -0.02413(17) 0.40718(13) 0.22363(7) 1.000 0.0271(5) . .
C223 C Uani -0.14920(19) 0.44372(13) 0.22458(9) 1.000 0.0326(6) . .
C224 C Uani -0.23257(17) 0.43774(12) 0.18418(9) 1.000 0.0303(6) . .
C225 C Uani -0.19424(17) 0.39506(12) 0.14113(8) 1.000 0.0279(5) . .
C226 C Uani -0.07015(16) 0.35815(12) 0.13925(7) 1.000 0.0226(5) . .
C227 C Uani -0.00793(18) 0.30345(15) 0.09941(8) 1.000 0.0306(6) . .
C228 C Uani 0.13539(17) 0.29597(13) 0.11706(7) 1.000 0.0245(5) . .


H22 H Uiso 0.30274 0.11461 0.27323 1.00(4) 0.029(2) . .
H23 H Uiso 0.50614 0.05834 0.30709 1.00(4) 0.035(2) . .
H25 H Uiso 0.74284 0.04430 0.30924 1.00(4) 0.044(2) . .
H26 H Uiso 0.95225 0.08515 0.27577 1.00(4) 0.025(2) . .
H27 H Uiso 0.96164 0.18509 0.20772 1.00(4) 0.021(2) . .
H28 H Uiso 0.77055 0.23373 0.17214 1.00(4) 0.0214(19) . .
H213 H Uiso 0.63333 0.10446 0.12355 1.00(4) 0.023(2) . .
H214 H Uiso 0.73254 0.06968 0.05286 1.00(3) 0.0164(19) . .
H215 H Uiso 0.76715 0.17209 -0.01263 1.00(4) 0.040(2) . .
H216 H Uiso 0.65534 0.30339 -0.01253 1.00(4) 0.035(2) . .
H218 H Uiso 0.52374 0.39743 0.03861 1.00(3) 0.0186(19) . .
H219 H Uiso 0.41670 0.43704 0.11016 1.00(4) 0.024(2) . .
H222 H Uiso 0.02692 0.40424 0.25526 1.00(3) 0.0071(16) . .
H223 H Uiso -0.17967 0.47767 0.25399 1.00(4) 0.034(2) . .
H224 H Uiso -0.31701 0.46151 0.18647 1.00(4) 0.034(2) . .
H225 H Uiso -0.25565 0.39212 0.11048 1.00(4) 0.038(2) . .
H227 H Uiso -0.01906 0.33099 0.06474 1.00(4) 0.034(2) . .
H227' H Uiso -0.05264 0.23909 0.10133 1.00(6) 0.075(3) . .
H228 H Uiso 0.18130 0.23654 0.11528 1.00(4) 0.026(2) . .
H228' H Uiso 0.19013 0.33627 0.09671 1.00(4) 0.031(2) . .


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_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
P1 0.0196(2) 0.0207(2) 0.0206(2) -0.0053(2) -0.0033(2) 0.0043(2)
O11 0.0276(6) 0.0199(6) 0.0162(5) -0.0023(5) -0.0006(5) 0.0039(5)
O12 0.0230(6) 0.0185(6) 0.0215(6) -0.0007(5) -0.0015(5) 0.0041(5)
N1 0.0201(7) 0.0322(9) 0.0262(7) -0.0100(7) -0.0045(6) 0.0054(6)
C11 0.0251(8) 0.0185(8) 0.0169(8) 0.0003(7) 0.0011(6) 0.0035(7)
C12 0.0303(9) 0.0261(10) 0.0230(9) 0.0012(8) 0.0097(7) 0.0003(7)
C13 0.0271(9) 0.0243(10) 0.0324(10) 0.0038(8) 0.0099(8) -0.0060(7)
C14 0.0222(8) 0.0161(8) 0.0278(9) 0.0010(7) 0.0011(7) -0.0001(6)
C15 0.0250(8) 0.0158(9) 0.0346(10) -0.0008(8) -0.0017(7) -0.0041(7)
```

```
C16 0.0305(9) 0.0181(9) 0.0303(9) -0.0057(8) -0.0086(8) 0.0016(7)
C17 0.0292(9) 0.0220(9) 0.0191(8) -0.0006(7) -0.0026(7) 0.0050(7)
C18 0.0211(7) 0.0181(8) 0.0193(8) 0.0006(7) 0.0009(6) 0.0008(7)
C19 0.0203(7) 0.0144(8) 0.0191(8) 0.0018(7) -0.0002(6) 0.0022(6)
C110 0.0213(7) 0.0127(8) 0.0175(8) 0.0005(6) 0.0001(6) 0.0029(6)
C111 0.0194(7) 0.0175(8) 0.0131(7) 0.0012(6) -0.0026(6) 0.0007(6)
C112 0.0214(7) 0.0222(9) 0.0128(7) 0.0022(6) -0.0024(6) 0.0014(6)
C113 0.0275(8) 0.0233(9) 0.0185(8) 0.0005(7) -0.0016(7) 0.0036(7)
C114 0.0331(10) 0.0301(11) 0.0251(9) -0.0017(8) 0.0008(8) 0.0123(8)
C115 0.0221(8) 0.0492(13) 0.0242(9) 0.0019(9) 0.0049(7) 0.0093(8)
C116 0.0213(8) 0.0409(11) 0.0202(8) 0.0039(8) 0.0010(7) -0.0010(8)
C117 0.0214(8) 0.0299(10) 0.0152(7) 0.0020(7) -0.0018(6) -0.0013(7)
C118 0.0245(8) 0.0258(10) 0.0214(8) 0.0033(7) -0.0054(7) -0.0071(7)
C119 0.0286(9) 0.0148(9) 0.0252(9) 0.0007(7) -0.0066(7) -0.0022(7)
C120 0.0191(7) 0.0219(8) 0.0171(7) 0.0003(6) -0.0023(6) 0.0013(7)
C121 0.0241(8) 0.0153(8) 0.0233(8) 0.0012(7) 0.0031(7) 0.0015(6)
C122 0.0284(9) 0.0223(10) 0.0274(9) -0.0043(8) -0.0014(7) 0.0044(7)
C123 0.0411(11) 0.0245(10) 0.0298(10) -0.0082(8) 0.0070(9) 0.0002(8)
C124 0.0317(10) 0.0336(12) 0.0470(12) -0.0112(10) 0.0153(9) -0.0003(8)
C125 0.0228(9) 0.0359(12) 0.0509(13) -0.0032(10) 0.0068(9) 0.0024(8)
C126 0.0216(7) 0.0218(9) 0.0295(9) 0.0042(7) 0.0019(8) -0.0008(7)
C127 0.0199(8) 0.0402(11) 0.0316(10) 0.0001(9) -0.0026(7) -0.0032(8)
C128 0.0252(9) 0.0601(16) 0.0441(13) -0.0285(12) -0.0117(9) 0.0099(10)
P2 0.0165(2) 0.0254(2) 0.0188(2) -0.0005(2) 0.0002(2) 0.0013(2)
O21 0.0182(5) 0.0205(6) 0.0273(6) 0.0020(5) 0.0009(4) -0.0016(4)
O22 0.0190(5) 0.0194(6) 0.0248(6) -0.0007(5) 0.0016(5) -0.0003(5)
N2 0.0178(6) 0.0293(8) 0.0209(7) 0.0004(6) -0.0008(5) 0.0033(6)
C21 0.0207(7) 0.0175(8) 0.0219(8) -0.0009(7) -0.0002(6) -0.0009(6)
C22 0.0285(8) 0.0218(9) 0.0232(8) 0.0012(7) 0.0065(7) -0.0057(7)
C23 0.0340(9) 0.0203(9) 0.0177(8) 0.0027(7) 0.0014(7) -0.0027(7)
C24 0.0279(8) 0.0153(8) 0.0170(8) -0.0009(6) -0.0028(7) 0.0000(7)
C25 0.0369(9) 0.0167(8) 0.0202(8) 0.0016(7) -0.0071(8) 0.0038(8)
C26 0.0304(9) 0.0227(10) 0.0276(9) -0.0021(8) -0.0088(8) 0.0074(7)
C27 0.0215(8) 0.0235(9) 0.0297(9) -0.0013(8) -0.0046(7) 0.0014(7)
C28 0.0217(8) 0.0176(8) 0.0209(8) 0.0017(7) -0.0001(6) 0.0002(7)
C29 0.0233(8) 0.0132(8) 0.0167(7) -0.0020(6) -0.0016(6) -0.0008(6)
C210 0.0205(7) 0.0128(8) 0.0173(7) 0.0002(6) 0.0003(6) -0.0012(6)
C211 0.0136(6) 0.0185(8) 0.0195(8) 0.0029(6) -0.0014(6) -0.0016(6)
C212 0.0169(7) 0.0233(9) 0.0179(8) 0.0014(7) -0.0029(6) -0.0034(6)
C213 0.0232(8) 0.0287(10) 0.0217(8) -0.0039(8) -0.0019(7) -0.0008(7)
C214 0.0280(9) 0.0441(13) 0.0278(10) -0.0146(9) -0.0018(8) 0.0065(9)
C215 0.0293(10) 0.0675(16) 0.0176(9) -0.0097(10) 0.0034(7) 0.0015(10)
C216 0.0304(9) 0.0510(14) 0.0194(9) 0.0017(9) 0.0004(7) -0.0055(9)
C217 0.0204(8) 0.0342(10) 0.0169(8) 0.0027(7) -0.0038(6) -0.0064(7)
C218 0.0241(8) 0.0297(10) 0.0242(9) 0.0139(8) -0.0080(7) -0.0075(8)
C219 0.0179(8) 0.0205(9) 0.0321(10) 0.0067(8) -0.0056(7) -0.0012(7)
C220 0.0134(7) 0.0209(9) 0.0234(8) -0.0003(7) -0.0025(6) -0.0021(6)
C221 0.0164(7) 0.0190(9) 0.0267(8) 0.0026(7) 0.0032(7) -0.0018(6)
C222 0.0235(8) 0.0267(10) 0.0310(10) -0.0035(8) 0.0029(7) -0.0008(7)
C223 0.0253(9) 0.0255(10) 0.0470(12) -0.0076(9) 0.0077(8) 0.0010(8)
C224 0.0171(8) 0.0198(9) 0.0540(13) 0.0025(9) 0.0057(8) 0.0015(7)
C225 0.0198(8) 0.0200(9) 0.0440(11) 0.0061(9) -0.0059(8) -0.0034(7)
C226 0.0178(7) 0.0200(9) 0.0301(9) 0.0017(8) -0.0007(7) -0.0042(6)
C227 0.0227(8) 0.0418(12) 0.0272(9) -0.0041(9) -0.0041(7) -0.0011(8)
C228 0.0233(8) 0.0285(10) 0.0217(8) -0.0048(8) -0.0030(7) 0.0026(7)

#=============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All esds are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
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 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 P1      O11      1.6423(13)                    .       .                 yes
 P1      O12      1.6639(12)                    .       .                 yes
 P1      N1       1.6659(15)                    .       .                 yes
 P2      O22      1.6572(12)                    .       .                 yes
 P2      N2       1.6670(14)                    .       .                 yes
 P2      O21      1.6599(13)                    .       .                 yes
 O11     C11        1.400(2)                    .       .                 yes
 O12     C120       1.398(2)                    .       .                 yes
 O21     C21        1.396(2)                    .       .                 yes
 O22     C220     1.3948(19)                    .       .                 yes
 N1      C128       1.495(3)                    .       .                 yes
 N1      C121       1.409(2)                    .       .                 yes
 N2      C228       1.493(2)                    .       .                 yes
 N2      C221       1.414(2)                    .       .                 yes
 C11     C12        1.409(3)                    .       .                 no
 C11     C110       1.379(2)                    .       .                 no
 C12     C13        1.364(3)                    .       .                 no
 C13     C14        1.417(3)                    .       .                 no
 C14     C15        1.416(3)                    .       .                 no
 C14     C19        1.426(2)                    .       .                 no
 C15     C16        1.364(3)                    .       .                 no
 C16     C17        1.404(3)                    .       .                 no
 C17     C18        1.374(2)                    .       .                 no
 C18     C19        1.419(2)                    .       .                 no
 C19     C110       1.439(2)                    .       .                 no
 C110    C111       1.490(2)                    .       .                 no
 C111    C112       1.442(2)                    .       .                 no
 C111    C120       1.377(2)                    .       .                 no
 C112    C113       1.420(3)                    .       .                 no
 C112    C117       1.427(2)                    .       .                 no
 C12     H12          0.9840                    .       .                 no
 C13     H13          0.9821                    .       .                 no
 C113    C114       1.374(3)                    .       .                 no
 C114    C115       1.404(3)                    .       .                 no
 C15     H15          0.8972                    .       .                 no
 C115    C116       1.364(3)                    .       .                 no
 C16     H16          0.9227                    .       .                 no
 C116    C117       1.422(2)                    .       .                 no
 C17     H17          0.9437                    .       .                 no
 C117    C118       1.411(3)                    .       .                 no
 C118    C119       1.367(3)                    .       .                 no
 C18     H18          0.9180                    .       .                 no
 C119    C120       1.408(2)                    .       .                 no
 C121    C122       1.386(3)                    .       .                 no
 C121    C126       1.395(2)                    .       .                 no
 C122    C123       1.398(3)                    .       .                 no
 C123    C124       1.383(3)                    .       .                 no
 C124    C125       1.383(3)                    .       .                 no
 C125    C126       1.388(3)                    .       .                 no
 C126    C127       1.505(3)                    .       .                 no
 C127    C128       1.511(3)                    .       .                 no
 C113    H113         0.9628                    .       .                 no
 C114    H114         0.9196                    .       .                 no
 C115    H115         0.9760                    .       .                 no
 C116    H116         0.9722                    .       .                 no
 C118    H118         0.9408                    .       .                 no
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 C119    H119         0.9362                    .      .                 no
 C21     C22        1.413(2)                    .      .                 no
 C21     C210       1.375(2)                    .      .                 no
 C22     C23        1.364(3)                    .      .                 no
 C122    H122         0.9282                    .      .                 no
 C23     C24        1.420(3)                    .      .                 no
 C123    H123         0.9696                    .      .                 no
 C24     C25        1.419(3)                    .      .                 no
 C124    H124         0.9024                    .      .                 no
 C24     C29        1.433(2)                    .      .                 no
 C25     C26        1.356(3)                    .      .                 no
 C125    H125         1.0131                    .      .                 no
 C26     C27        1.413(3)                    .      .                 no
 C127    H127'        1.0596                    .      .                 no
 C127    H127         0.9264                    .      .                 no
 C27     C28        1.368(2)                    .      .                 no
 C128    H128'        1.1083                    .      .                 no
 C128    H128         0.9345                    .      .                 no
 C28     C29        1.416(2)                    .      .                 no
 C29     C210       1.436(2)                    .      .                 no
 C22     H22          1.0154                    .      .                 no
 C23     H23          0.9087                    .      .                 no
 C25     H25          0.9930                    .      .                 no
 C26     H26          0.9913                    .      .                 no
 C27     H27          1.0025                    .      .                 no
 C28     H28          0.9575                    .      .                 no
 C210    C211       1.495(2)                    .      .                 no
 C211    C212       1.435(2)                    .      .                 no
 C211    C220       1.380(2)                    .      .                 no
 C212    C217       1.431(3)                    .      .                 no
 C212    C213       1.419(3)                    .      .                 no
 C213    C214       1.377(3)                    .      .                 no
 C214    C215       1.415(3)                    .      .                 no
 C215    C216       1.363(4)                    .      .                 no
 C216    C217       1.414(3)                    .      .                 no
 C217    C218       1.419(3)                    .      .                 no
 C218    C219       1.359(3)                    .      .                 no
 C219    C220       1.408(3)                    .      .                 no
 C221    C222       1.389(3)                    .      .                 no
 C221    C226       1.389(2)                    .      .                 no
 C222    C223       1.399(3)                    .      .                 no
 C223    C224       1.375(3)                    .      .                 no
 C224    C225       1.386(3)                    .      .                 no
 C225    C226       1.393(2)                    .      .                 no
 C226    C227       1.508(3)                    .      .                 no
 C227    C228       1.539(3)                    .      .                 no
 C213    H213         0.9769                    .      .                 no
 C214    H214         0.9108                    .      .                 no
 C215    H215         0.8874                    .      .                 no
 C216    H216         1.0237                    .      .                 no
 C218    H218         0.8756                    .      .                 no
 C219    H219         0.9125                    .      .                 no
 C222    H222         0.9917                    .      .                 no
 C223    H223         0.9987                    .      .                 no
 C224    H224         0.9404                    .      .                 no
 C225    H225         1.0301                    .      .                 no
 C227    H227'        1.1133                    .      .                 no
 C227    H227         1.0273                    .      .                 no
 C228    H228'        1.0044                    .      .                 no
 C228    H228         1.0482                    .      .                 no

loop_
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_geom_angle_atom_site_label_3
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_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 O11     P1      O12        98.22(6)              .       .       .          yes
 O11     P1      N1        108.18(8)              .       .       .          yes
 O12     P1      N1         95.35(7)              .       .       .          yes
 O22     P2      N2        105.89(7)              .       .       .          yes
 O21     P2      O22        98.35(6)              .       .       .          yes
 O21     P2      N2         95.30(7)              .       .       .          yes
 P1      O11     C11       122.70(10)             .       .       .          yes
 P1      O12     C120      114.65(10)             .       .       .          yes
 P2      O21     C21       114.82(11)             .       .       .          yes
 P2      O22     C220      124.74(11)             .       .       .          yes
 C121    N1      C128      108.40(15)             .       .       .          yes
 P1      N1      C121      123.46(13)             .       .       .          yes
 P1      N1      C128      128.14(14)             .       .       .          yes
 P2      N2      C228      127.90(11)             .       .       .          yes
 C221    N2      C228      108.28(13)             .       .       .          yes
 P2      N2      C221      123.78(12)             .       .       .          yes
 C12     C11     C110      122.98(16)             .       .       .          no
 O11     C11     C12       116.48(14)             .       .       .          yes
 O11     C11     C110      120.51(15)             .       .       .          yes
 C11     C12     C13       119.19(17)             .       .       .          no
 C12     C13     C14       121.06(18)             .       .       .          no
 C13     C14     C19       119.42(16)             .       .       .          no
 C15     C14     C19       119.44(16)             .       .       .          no
 C13     C14     C15       121.12(16)             .       .       .          no
 C14     C15     C16       121.07(17)             .       .       .          no
 C15     C16     C17       119.79(17)             .       .       .          no
 C16     C17     C18       120.89(17)             .       .       .          no
 C17     C18     C19       120.84(16)             .       .       .          no
 C14     C19     C18       117.92(15)             .       .       .          no
 C14     C19     C110      119.25(15)             .       .       .          no
 C18     C19     C110      122.75(15)             .       .       .          no
 C11     C110    C19       117.83(15)             .       .       .          no
 C11     C110    C111      119.37(15)             .       .       .          no
 C19     C110    C111      122.67(14)             .       .       .          no
 C110    C111    C112      123.44(15)             .       .       .          no
 C112    C111    C120      117.80(15)             .       .       .          no
 C110    C111    C120      118.70(14)             .       .       .          no
 C111    C112    C117      118.85(15)             .       .       .          no
 C113    C112    C117      118.09(15)             .       .       .          no
 C111    C112    C113      123.01(15)             .       .       .          no
 C13     C12     H12           119.57             .       .       .          no
 C11     C12     H12           121.19             .       .       .          no
 C14     C13     H13           112.71             .       .       .          no
 C112    C113    C114      120.69(18)             .       .       .          no
 C12     C13     H13           126.23             .       .       .          no
 C113    C114    C115        121.1(2)             .       .       .          no
 C14     C15     H15           117.99             .       .       .          no
 C114    C115    C116      119.89(18)             .       .       .          no
 C16     C15     H15           120.75             .       .       .          no
 C17     C16     H16           123.27             .       .       .          no
 C15     C16     H16           116.78             .       .       .          no
 C115    C116    C117      120.93(18)             .       .       .          no
 C112    C117    C118      120.14(15)             .       .       .          no
 C112    C117    C116      119.31(17)             .       .       .          no
 C18     C17     H17           119.87             .       .       .          no
 C116    C117    C118      120.54(17)             .       .       .          no
 C16     C17     H17           119.21             .       .       .          no
 C17     C18     H18           121.41             .       .       .          no
 C19     C18     H18           117.70             .       .       .          no
 C117    C118    C119      120.50(16)             .       .       .          no
 C118    C119    C120      119.35(16)             .       .       .          no
 O12     C120    C119      117.12(15)             .       .       .          yes
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| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O12 | C120 | C111 | 119.63(14) | . | . | . | yes |
| C111 | C120 | C119 | 123.21(15) | . | . | . | no |
| N1 | C121 | C126 | 109.92(15) | . | . | . | yes |
| C122 | C121 | C126 | 120.84(16) | . | . | . | no |
| N1 | C121 | C122 | 129.24(16) | . | . | . | yes |
| C121 | C122 | C123 | 118.20(18) | . | . | . | no |
| C122 | C123 | C124 | 121.2(2) | . | . | . | no |
| C123 | C124 | C125 | 120.1(2) | . | . | . | no |
| C124 | C125 | C126 | 119.65(18) | . | . | . | no |
| C121 | C126 | C125 | 120.01(17) | . | . | . | no |
| C125 | C126 | C127 | 130.37(17) | . | . | . | no |
| C121 | C126 | C127 | 109.57(15) | . | . | . | no |
| C126 | C127 | C128 | 103.55(17) | . | . | . | no |
| N1 | C128 | C127 | 104.9(2) | . | . | . | yes |
| C114 | C113 | H113 | 119.62 | . | . | . | no |
| C112 | C113 | H113 | 119.69 | . | . | . | no |
| C113 | C114 | H114 | 117.59 | . | . | . | no |
| C115 | C114 | H114 | 121.28 | . | . | . | no |
| C116 | C115 | H115 | 121.42 | . | . | . | no |
| C114 | C115 | H115 | 118.68 | . | . | . | no |
| C117 | C116 | H116 | 121.88 | . | . | . | no |
| C115 | C116 | H116 | 117.19 | . | . | . | no |
| C119 | C118 | H118 | 123.63 | . | . | . | no |
| C117 | C118 | H118 | 115.79 | . | . | . | no |
| C118 | C119 | H119 | 120.90 | . | . | . | no |
| C120 | C119 | H119 | 119.66 | . | . | . | no |
| O21 | C21 | C22 | 117.86(15) | . | . | . | yes |
| O21 | C21 | C210 | 118.88(14) | . | . | . | yes |
| C22 | C21 | C210 | 123.25(16) | . | . | . | no |
| C123 | C122 | H122 | 118.16 | . | . | . | no |
| C121 | C122 | H122 | 123.51 | . | . | . | no |
| C21 | C22 | C23 | 119.20(17) | . | . | . | no |
| C122 | C123 | H123 | 120.70 | . | . | . | no |
| C22 | C23 | C24 | 120.91(17) | . | . | . | no |
| C124 | C123 | H123 | 117.86 | . | . | . | no |
| C23 | C24 | C25 | 121.59(16) | . | . | . | no |
| C23 | C24 | C29 | 119.24(15) | . | . | . | no |
| C123 | C124 | H124 | 118.54 | . | . | . | no |
| C125 | C124 | H124 | 121.37 | . | . | . | no |
| C25 | C24 | C29 | 119.12(16) | . | . | . | no |
| C124 | C125 | H125 | 121.29 | . | . | . | no |
| C126 | C125 | H125 | 119.05 | . | . | . | no |
| C24 | C25 | C26 | 121.33(17) | . | . | . | no |
| C25 | C26 | C27 | 119.87(17) | . | . | . | no |
| C126 | C127 | H127' | 109.68 | . | . | . | no |
| C126 | C127 | H127 | 114.34 | . | . | . | no |
| C128 | C127 | H127' | 111.89 | . | . | . | no |
| C26 | C27 | C28 | 120.38(16) | . | . | . | no |
| C128 | C127 | H127 | 113.11 | . | . | . | no |
| H127' | C127 | H127 | 104.44 | . | . | . | no |
| H128' | C128 | H128 | 103.13 | . | . | . | no |
| C127 | C128 | H128' | 110.54 | . | . | . | no |
| C127 | C128 | H128 | 119.52 | . | . | . | no |
| N1 | C128 | H128' | 111.23 | . | . | . | no |
| N1 | C128 | H128 | 107.55 | . | . | . | no |
| C27 | C28 | C29 | 121.56(16) | . | . | . | no |
| C24 | C29 | C28 | 117.58(15) | . | . | . | no |
| C24 | C29 | C210 | 119.39(15) | . | . | . | no |
| C28 | C29 | C210 | 122.95(15) | . | . | . | no |
| C23 | C22 | H22 | 125.84 | . | . | . | no |
| C21 | C22 | H22 | 114.86 | . | . | . | no |
| C22 | C23 | H23 | 121.12 | . | . | . | no |
| C24 | C23 | H23 | 117.96 | . | . | . | no |
| C26 | C25 | H25 | 121.57 | . | . | . | no |
| C24 | C25 | H25 | 117.00 | . | . | . | no |
| C25 | C26 | H26 | 121.92 | . | . | . | no |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C27 | C26 | H26 | 118.21 | . | . | . | no |
| C26 | C27 | H27 | 121.42 | . | . | . | no |
| C28 | C27 | H27 | 118.20 | . | . | . | no |
| C29 | C28 | H28 | 119.96 | . | . | . | no |
| C27 | C28 | H28 | 118.38 | . | . | . | no |
| C21 | C210 | C211 | 119.79(14) | . | . | . | no |
| C21 | C210 | C29 | 117.79(15) | . | . | . | no |
| C29 | C210 | C211 | 122.36(14) | . | . | . | no |
| C212 | C211 | C220 | 117.95(15) | . | . | . | no |
| C210 | C211 | C212 | 122.28(15) | . | . | . | no |
| C210 | C211 | C220 | 119.77(14) | . | . | . | no |
| C211 | C212 | C213 | 122.17(16) | . | . | . | no |
| C211 | C212 | C217 | 119.45(16) | . | . | . | no |
| C213 | C212 | C217 | 118.36(15) | . | . | . | no |
| C212 | C213 | C214 | 120.62(18) | . | . | . | no |
| C213 | C214 | C215 | 120.2(2) | . | . | . | no |
| C214 | C215 | C216 | 120.52(19) | . | . | . | no |
| C215 | C216 | C217 | 120.6(2) | . | . | . | no |
| C216 | C217 | C218 | 121.51(19) | . | . | . | no |
| C212 | C217 | C216 | 119.37(18) | . | . | . | no |
| C212 | C217 | C218 | 119.11(16) | . | . | . | no |
| C217 | C218 | C219 | 120.82(18) | . | . | . | no |
| C218 | C219 | C220 | 119.90(17) | . | . | . | no |
| O22 | C220 | C211 | 120.76(14) | . | . | . | yes |
| O22 | C220 | C219 | 116.56(15) | . | . | . | yes |
| C211 | C220 | C219 | 122.53(15) | . | . | . | no |
| N2 | C221 | C226 | 110.75(15) | . | . | . | yes |
| C222 | C221 | C226 | 121.49(15) | . | . | . | no |
| N2 | C221 | C222 | 127.72(16) | . | . | . | yes |
| C221 | C222 | C223 | 117.63(17) | . | . | . | no |
| C222 | C223 | C224 | 121.4(2) | . | . | . | no |
| C223 | C224 | C225 | 120.50(17) | . | . | . | no |
| C224 | C225 | C226 | 119.23(18) | . | . | . | no |
| C225 | C226 | C227 | 130.24(17) | . | . | . | no |
| C221 | C226 | C227 | 109.86(15) | . | . | . | no |
| C221 | C226 | C225 | 119.77(17) | . | . | . | no |
| C226 | C227 | C228 | 103.15(16) | . | . | . | no |
| N2 | C228 | C227 | 104.96(14) | . | . | . | yes |
| C212 | C213 | H213 | 119.06 | . | . | . | no |
| C214 | C213 | H213 | 120.23 | . | . | . | no |
| C213 | C214 | H214 | 111.67 | . | . | . | no |
| C215 | C214 | H214 | 127.87 | . | . | . | no |
| C214 | C215 | H215 | 118.50 | . | . | . | no |
| C216 | C215 | H215 | 120.88 | . | . | . | no |
| C215 | C216 | H216 | 121.65 | . | . | . | no |
| C217 | C216 | H216 | 117.62 | . | . | . | no |
| C217 | C218 | H218 | 117.35 | . | . | . | no |
| C219 | C218 | H218 | 121.82 | . | . | . | no |
| C218 | C219 | H219 | 120.38 | . | . | . | no |
| C220 | C219 | H219 | 119.55 | . | . | . | no |
| C221 | C222 | H222 | 122.80 | . | . | . | no |
| C223 | C222 | H222 | 118.80 | . | . | . | no |
| C222 | C223 | H223 | 121.21 | . | . | . | no |
| C224 | C223 | H223 | 117.36 | . | . | . | no |
| C223 | C224 | H224 | 119.15 | . | . | . | no |
| C225 | C224 | H224 | 120.32 | . | . | . | no |
| C224 | C225 | H225 | 120.48 | . | . | . | no |
| C226 | C225 | H225 | 120.27 | . | . | . | no |
| C226 | C227 | H227' | 108.47 | . | . | . | no |
| C226 | C227 | H227 | 110.21 | . | . | . | no |
| C228 | C227 | H227' | 107.73 | . | . | . | no |
| C228 | C227 | H227 | 114.34 | . | . | . | no |
| H227' | C227 | H227 | 112.41 | . | . | . | no |
| N2 | C228 | H228' | 110.53 | . | . | . | no |
| N2 | C228 | H228 | 107.40 | . | . | . | no |
| C227 | C228 | H228' | 108.26 | . | . | . | no |

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 C227    C228    H228         118.57             .       .       .          no
 H228'   C228    H228         107.04             .       .       .          no

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 O12     P1      O11     C11       37.04(13)     .       .       .       .   no
 N1      P1      O11     C11      -61.39(14)     .       .       .       .   no
 O11     P1      O12     C120      55.53(12)     .       .       .       .   no
 N1      P1      O12     C120     164.81(12)     .       .       .       .   no
 O11     P1      N1      C121    -123.64(15)     .       .       .       .   no
 O11     P1      N1      C128        55.3(2)     .       .       .       .   no
 O12     P1      N1      C121     135.88(15)     .       .       .       .   no
 O12     P1      N1      C128       -45.1(2)     .       .       .       .   no
 O21     P2      N2      C221     138.86(14)     .       .       .       .   no
 O21     P2      N2      C228     -43.80(16)     .       .       .       .   no
 O22     P2      N2      C221    -120.88(14)     .       .       .       .   no
 O22     P2      O21     C21       58.68(12)     .       .       .       .   no
 N2      P2      O21     C21      165.64(11)     .       .       .       .   no
 O21     P2      O22     C220      32.76(13)     .       .       .       .   no
 N2      P2      O22     C220     -65.22(14)     .       .       .       .   no
 O22     P2      N2      C228      56.45(17)     .       .       .       .   no
 P1      O11     C11     C110     -71.92(19)     .       .       .       .   no
 P1      O11     C11     C12      110.09(16)     .       .       .       .   no
 P1      O12     C120    C111     -82.34(16)     .       .       .       .   no
 P1      O12     C120    C119      99.64(16)     .       .       .       .   no
 P2      O21     C21     C210     -81.93(17)     .       .       .       .   no
 P2      O21     C21     C22       99.49(16)     .       .       .       .   no
 P2      O22     C220    C211     -67.25(18)     .       .       .       .   no
 P2      O22     C220    C219     117.05(15)     .       .       .       .   no
 P1      N1      C128    C127     163.22(15)     .       .       .       .   no
 C121    N1      C128    C127       -17.7(2)     .       .       .       .   no
 C128    N1      C121    C126         9.2(2)     .       .       .       .   no
 P1      N1      C121    C122         7.7(3)     .       .       .       .   no
 P1      N1      C121    C126    -171.69(14)     .       .       .       .   no
 C128    N1      C121    C122      -171.4(2)     .       .       .       .   no
 C228    N2      C221    C222    -173.42(18)     .       .       .       .   no
 P2      N2      C228    C227     166.28(14)     .       .       .       .   no
 P2      N2      C221    C226    -173.56(13)     .       .       .       .   no
 C228    N2      C221    C226         8.7(2)     .       .       .       .   no
 P2      N2      C221    C222         4.4(3)     .       .       .       .   no
 C221    N2      C228    C227       -16.0(2)     .       .       .       .   no
 C12     C11     C110    C111     178.05(16)     .       .       .       .   no
 O11     C11     C110    C19      176.16(14)     .       .       .       .   no
 O11     C11     C110    C111         0.2(2)     .       .       .       .   no
 C110    C11     C12     C13          2.5(3)     .       .       .       .   no
 C12     C11     C110    C19         -6.0(3)     .       .       .       .   no
 O11     C11     C12     C13     -179.54(17)     .       .       .       .   no
 C11     C12     C13     C14          1.9(3)     .       .       .       .   no
 C12     C13     C14     C19         -2.5(3)     .       .       .       .   no
 C12     C13     C14     C15      175.69(18)     .       .       .       .   no
 C13     C14     C15     C16     -176.70(18)     .       .       .       .   no
 C15     C14     C19     C110    -179.29(16)     .       .       .       .   no
 C19     C14     C15     C16          1.5(3)     .       .       .       .   no
 C15     C14     C19     C18         -2.3(2)     .       .       .       .   no
 C13     C14     C19     C18      175.99(16)     .       .       .       .   no
 C13     C14     C19     C110        -1.0(2)     .       .       .       .   no
 C14     C15     C16     C17          0.3(3)     .       .       .       .   no
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| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C15 | C16 | C17 | C18 | -1.3(3) | . | . | . | no |
| C16 | C17 | C18 | C19 | 0.5(3) | . | . | . | no |
| C17 | C18 | C19 | C14 | 1.3(2) | . | . | . | no |
| C17 | C18 | C19 | C110 | 178.18(16) | . | . | . | no |
| C18 | C19 | C110 | C111 | 4.1(2) | . | . | . | no |
| C14 | C19 | C110 | C111 | -179.06(15) | . | . | . | no |
| C18 | C19 | C110 | C11 | -171.76(16) | . | . | . | no |
| C14 | C19 | C110 | C11 | 5.1(2) | . | . | . | no |
| C111 | C112 | C113 | H113 | -0.03 | . | . | . | no |
| C117 | C112 | C113 | H113 | -177.28 | . | . | . | no |
| H113 | C113 | C114 | H114 | 1.27 | . | . | . | no |
| C112 | C113 | C114 | H114 | -177.88 | . | . | . | no |
| H113 | C113 | C114 | C115 | 178.33 | . | . | . | no |
| C113 | C114 | C115 | H115 | 179.37 | . | . | . | no |
| H114 | C114 | C115 | C116 | 176.70 | . | . | . | no |
| H114 | C114 | C115 | H115 | -3.67 | . | . | . | no |
| C114 | C115 | C116 | H116 | -178.82 | . | . | . | no |
| H115 | C115 | C116 | H116 | 1.56 | . | . | . | no |
| H115 | C115 | C116 | C117 | -179.41 | . | . | . | no |
| H116 | C116 | C117 | C112 | 179.87 | . | . | . | no |
| H116 | C116 | C117 | C118 | 0.75 | . | . | . | no |
| C112 | C117 | C118 | H118 | 179.95 | . | . | . | no |
| C116 | C117 | C118 | H118 | -0.94 | . | . | . | no |
| H118 | C118 | C119 | C120 | 179.69 | . | . | . | no |
| H118 | C118 | C119 | H119 | -3.80 | . | . | . | no |
| C117 | C118 | C119 | H119 | 179.41 | . | . | . | no |
| H119 | C119 | C120 | O12 | 1.83 | . | . | . | no |
| H119 | C119 | C120 | C111 | -176.10 | . | . | . | no |
| C210 | C21 | C22 | C23 | 0.3(3) | . | . | . | no |
| O21 | C21 | C22 | C23 | 178.81(16) | . | . | . | no |
| N1 | C121 | C122 | H122 | 2.93 | . | . | . | no |
| O21 | C21 | C210 | C29 | 177.41(14) | . | . | . | no |
| C22 | C21 | C210 | C211 | 178.64(16) | . | . | . | no |
| C22 | C21 | C210 | C29 | -4.1(3) | . | . | . | no |
| O21 | C21 | C210 | C211 | 0.1(3) | . | . | . | no |
| C126 | C121 | C122 | H122 | -177.69 | . | . | . | no |
| H122 | C122 | C123 | H123 | 2.14 | . | . | . | no |
| H122 | C122 | C123 | C124 | 176.80 | . | . | . | no |
| C121 | C122 | C123 | H123 | -173.76 | . | . | . | no |
| C21 | C22 | C23 | C24 | 1.9(3) | . | . | . | no |
| H123 | C123 | C124 | H124 | -2.31 | . | . | . | no |
| H123 | C123 | C124 | C125 | 175.51 | . | . | . | no |
| C22 | C23 | C24 | C25 | 177.37(18) | . | . | . | no |
| C122 | C123 | C124 | H124 | -177.11 | . | . | . | no |
| C22 | C23 | C24 | C29 | -0.1(3) | . | . | . | no |
| C23 | C24 | C29 | C210 | -3.7(2) | . | . | . | no |
| C29 | C24 | C25 | C26 | 3.2(3) | . | . | . | no |
| C23 | C24 | C29 | C28 | 172.96(16) | . | . | . | no |
| C123 | C124 | C125 | H125 | 177.50 | . | . | . | no |
| C23 | C24 | C25 | C26 | -174.27(18) | . | . | . | no |
| H124 | C124 | C125 | C126 | 176.58 | . | . | . | no |
| H124 | C124 | C125 | H125 | -4.74 | . | . | . | no |
| C25 | C24 | C29 | C210 | 178.73(16) | . | . | . | no |
| C25 | C24 | C29 | C28 | -4.6(2) | . | . | . | no |
| H125 | C125 | C126 | C121 | -178.65 | . | . | . | no |
| C24 | C25 | C26 | C27 | 0.3(3) | . | . | . | no |
| H125 | C125 | C126 | C127 | -1.52 | . | . | . | no |
| C125 | C126 | C127 | H127' | -71.89 | . | . | . | no |
| C121 | C126 | C127 | H127 | -137.61 | . | . | . | no |
| C25 | C26 | C27 | C28 | -2.4(3) | . | . | . | no |
| C121 | C126 | C127 | H127' | 105.48 | . | . | . | no |
| C125 | C126 | C127 | H127 | 45.02 | . | . | . | no |
| H127 | C127 | C128 | H128 | -96.41 | . | . | . | no |
| H127 | C127 | C128 | N1 | 142.98 | . | . | . | no |
| H127' | C127 | C128 | H128' | 140.63 | . | . | . | no |
| H127' | C127 | C128 | H128 | 21.22 | . | . | . | no |

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 H127    C127    C128    H128'         23.00     .       .       .       .   no
 C126    C127    C128    H128'       -101.32     .       .       .       .   no
 C126    C127    C128    H128         139.27     .       .       .       .   no
 C26     C27     C28     C29           0.8(3)    .       .       .       .   no
 H127'   C127    C128    N1           -99.38     .       .       .       .   no
 C27     C28     C29     C24           2.6(2)    .       .       .       .   no
 C27     C28     C29     C210      179.19(17)    .       .       .       .   no
 C28     C29     C210    C211          6.4(3)    .       .       .       .   no
 C24     C29     C210    C21           5.7(2)    .       .       .       .   no
 C28     C29     C210    C21      -170.79(16)    .       .       .       .   no
 C24     C29     C210    C211     -177.10(15)    .       .       .       .   no
 C29     C210    C211    C220     -126.20(17)    .       .       .       .   no
 C21     C210    C211    C212     -129.08(17)    .       .       .       .   no
 C29     C210    C211    C212         53.8(2)    .       .       .       .   no
 C21     C210    C211    C220         50.9(2)    .       .       .       .   no
 C220    C211    C212    C213     -172.80(16)    .       .       .       .   no
 C220    C211    C212    C217          5.7(2)    .       .       .       .   no
 C210    C211    C212    C217     -174.23(15)    .       .       .       .   no
 C210    C211    C220    C219      174.48(15)    .       .       .       .   no
 C212    C211    C220    O22       179.07(14)    .       .       .       .   no
 C210    C211    C220    O22          -1.0(2)    .       .       .       .   no
 C210    C211    C212    C213          7.2(2)    .       .       .       .   no
 C212    C211    C220    C219         -5.5(2)    .       .       .       .   no
 C211    C212    C213    C214     -176.40(17)    .       .       .       .   no
 C217    C212    C213    C214          5.0(3)    .       .       .       .   no
 C211    C212    C217    C216      176.05(17)    .       .       .       .   no
 C211    C212    C217    C218         -2.9(2)    .       .       .       .   no
 C213    C212    C217    C216         -5.4(3)    .       .       .       .   no
 C213    C212    C217    C218      175.69(16)    .       .       .       .   no
 C212    C213    C214    C215         -1.1(3)    .       .       .       .   no
 C213    C214    C215    C216         -2.6(3)    .       .       .       .   no
 C214    C215    C216    C217          2.2(3)    .       .       .       .   no
 C215    C216    C217    C212          1.8(3)    .       .       .       .   no
 C215    C216    C217    C218     -179.27(19)    .       .       .       .   no
 C216    C217    C218    C219     -179.36(18)    .       .       .       .   no
 C212    C217    C218    C219         -0.4(3)    .       .       .       .   no
 C217    C218    C219    C220          0.9(3)    .       .       .       .   no
 C218    C219    C220    O22       177.85(15)    .       .       .       .   no
 C218    C219    C220    C211          2.2(3)    .       .       .       .   no
 N2      C221    C222    C223     -178.76(18)    .       .       .       .   no
 C226    C221    C222    C223         -1.0(3)    .       .       .       .   no
 N2      C221    C226    C225      179.11(16)    .       .       .       .   no
 N2      C221    C226    C227          2.8(2)    .       .       .       .   no
 C222    C221    C226    C225          1.0(3)    .       .       .       .   no
 C222    C221    C226    C227     -175.30(18)    .       .       .       .   no
 C221    C222    C223    C224          0.6(3)    .       .       .       .   no
 C222    C223    C224    C225         -0.1(3)    .       .       .       .   no
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 C224    C225    C226    C227        175.0(2)    .       .       .       .   no
 C224    C225    C226    C221         -0.5(3)    .       .       .       .   no
 C221    C226    C227    C228        -12.4(2)    .       .       .       .   no
 C225    C226    C227    C228        171.7(2)    .       .       .       .   no
 C226    C227    C228    N2           16.8(2)    .       .       .       .   no

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 P1      H122          2.9954                    .       .                 no
 P1      H13           3.0282                    .     3_465               no
 P2      H222          2.9408                    .       .                 no
 O12     C219        3.347(2)                    .       .                 no
 O22     C17         3.396(2)                    .     4_645               no
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| | | | | | |
|---|---|---|---|---|---|
| O22 | C16 | 3.346(2) | . | 4_645 | no |
| O12 | H219 | 2.5749 | . | . | no |
| O12 | H128 | 2.5295 | . | . | no |
| O21 | H124 | 2.7853 | . | 3_455 | no |
| O21 | H228 | 2.4780 | . | . | no |
| O22 | H16 | 2.8719 | . | 4_645 | no |
| C11 | C128 | 3.324(3) | . | . | no |
| C12 | C128 | 3.412(3) | . | . | no |
| C16 | O22 | 3.346(2) | . | 4_655 | no |
| C17 | O22 | 3.396(2) | . | 4_655 | no |
| C18 | C113 | 3.176(2) | . | . | no |
| C18 | C112 | 3.283(2) | . | . | no |
| C18 | C24 | 3.494(2) | . | 4_655 | no |
| C19 | C113 | 3.293(2) | . | . | no |
| C24 | C18 | 3.494(2) | . | 4_645 | no |
| C26 | C222 | 3.535(3) | . | 4_645 | no |
| C26 | C117 | 3.471(2) | . | 4_645 | no |
| C28 | C225 | 3.564(3) | . | 1_655 | no |
| C28 | C212 | 3.221(2) | . | . | no |
| C28 | C226 | 3.491(2) | . | 1_655 | no |
| C28 | C213 | 3.110(2) | . | . | no |
| C29 | C213 | 3.210(2) | . | . | no |
| C11 | H128' | 2.9660 | . | . | no |
| C12 | H128' | 2.6245 | . | . | no |
| C12 | H127 | 2.8164 | . | 3_465 | no |
| C112 | C18 | 3.283(2) | . | . | no |
| C113 | C121 | 3.570(3) | . | 3_465 | no |
| C113 | C122 | 3.507(3) | . | 3_465 | no |
| C113 | C18 | 3.176(2) | . | . | no |
| C113 | C19 | 3.293(2) | . | . | no |
| C114 | C122 | 3.523(3) | . | 3_465 | no |
| C15 | H115 | 2.9760 | . | 1_655 | no |
| C117 | C26 | 3.471(2) | . | 4_655 | no |
| C118 | C127 | 3.503(3) | . | 1_455 | no |
| C18 | H113 | 2.7952 | . | . | no |
| C118 | C226 | 3.567(3) | . | . | no |
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| C21 | H124 | 2.9974 | . | 3_455 | no |
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| C22 | H224 | 3.0626 | . | 4_545 | no |
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| C122 | C113 | 3.507(3) | . | 3_565 | no |
| C23 | H16 | 2.9987 | . | 1_545 | no |
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| C28 | H213 | 2.7690 | . | . | no |
| C128 | C12 | 3.412(3) | . | . | no |
| C128 | C11 | 3.324(3) | . | . | no |
| C29 | H213 | 2.6446 | . | . | no |
| C110 | H113 | 2.7177 | . | . | no |
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| C212 | C28 | 3.221(2) | . | . | no |
| C113 | H18 | 2.7429 | . | . | no |
| C213 | C28 | 3.110(2) | . | . | no |
| C213 | C29 | 3.210(2) | . | . | no |
| C215 | C228 | 3.588(3) | . | 3_555 | no |
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| C117 | H12 | 3.0357 | . | 3_465 | no |
| C217 | C225 | 3.568(3) | . | 1_655 | no |
| C218 | C225 | 3.587(3) | . | 1_655 | no |
| C118 | H26 | 3.0566 | . | 4_655 | no |

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| C219 | C228 | 3.542(2) | . | . | no |
| C119 | H25 | 2.8902 | . | 4_655 | no |
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| C120 | H25 | 3.0650 | . | 4_655 | no |
| C220 | C228 | 3.345(2) | . | . | no |
| C121 | H113 | 2.9402 | . | 3_565 | no |
| C121 | H218 | 2.9515 | . | . | no |
| C222 | C26 | 3.535(3) | . | 4_655 | no |
| C122 | H114 | 2.9383 | . | 3_565 | no |
| C122 | H113 | 2.9163 | . | 3_565 | no |
| C123 | H228 | 2.7995 | . | 3_555 | no |
| C124 | H228 | 2.8424 | . | 3_555 | no |
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| C226 | C28 | 3.491(2) | . | 1_455 | no |
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| C228 | C215 | 3.588(3) | . | 3_455 | no |
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| C211 | H28 | 2.6946 | . | . | no |
| C212 | H28 | 2.6980 | . | . | no |
| C213 | H125 | 3.0520 | . | 3_455 | no |
| C213 | H28 | 2.8146 | . | . | no |
| C215 | H228' | 2.9661 | . | 3_555 | no |
| C217 | H225 | 2.7023 | . | 1_655 | no |
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| C218 | H215 | 2.9818 | . | 3_455 | no |
| C219 | H225 | 2.9654 | . | 1_655 | no |
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| C220 | H228' | 2.9784 | . | . | no |
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| C224 | H17 | 2.9162 | . | 4_545 | no |
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| C225 | H118 | 2.7691 | . | . | no |
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| H228' | C219 | 2.8048 | . | . | no |
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| H12 | C112 | 2.7845 | . | 3_565 | no |
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| H16 | C24 | 3.0093 | . | 1_565 | no |
| H16 | C23 | 2.9987 | . | 1_565 | no |

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| H17 | C223 | 3.0060 | . | 4_555 | no |
| H17 | C224 | 2.9162 | . | 4_555 | no |
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| H18 | C113 | 2.7429 | . | . | no |
| H18 | C111 | 2.6659 | . | . | no |
| H18 | C112 | 2.6948 | . | . | no |
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| H22 | H116 | 2.5355 | . | 4_545 | no |
| H22 | C224 | 3.0941 | . | 4_545 | no |
| H23 | H25 | 2.4226 | . | . | no |
| H23 | H224 | 2.4643 | . | 4_545 | no |
| H25 | H23 | 2.4226 | . | . | no |
| H25 | C119 | 2.8902 | . | 4_645 | no |
| H25 | C120 | 3.0650 | . | 4_645 | no |
| H26 | C117 | 3.0007 | . | 4_645 | no |
| H26 | C118 | 3.0566 | . | 4_645 | no |
| H26 | C222 | 2.8995 | . | 4_645 | no |
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| H27 | C221 | 2.9789 | . | 1_655 | no |
| H28 | C226 | 2.6925 | . | 1_655 | no |
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| H28 | C212 | 2.6980 | . | . | no |
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| H113 | C19 | 2.7337 | . | . | no |
| H113 | C110 | 2.7177 | . | . | no |
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| H114 | H122 | 2.4167 | . | 3_465 | no |
| H114 | C122 | 2.9383 | . | 3_465 | no |
| H115 | C15 | 2.9760 | . | 1_455 | no |
| H116 | H118 | 2.4331 | . | . | no |
| H116 | H22 | 2.5355 | . | 4_555 | no |
| H118 | C224 | 3.0817 | . | . | no |
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| H119 | H228' | 2.3956 | . | . | no |
| H122 | P1 | 2.9954 | . | . | no |
| H122 | H114 | 2.4167 | . | 3_565 | no |
| H124 | C21 | 2.9974 | . | 3_555 | no |
| H124 | O21 | 2.7853 | . | 3_555 | no |
| H125 | C213 | 3.0520 | . | 3_555 | no |
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| H127 | C12 | 2.8164 | . | 3_565 | no |
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| H213 | C28 | 2.7690 | . | . | no |
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| H213 | C210 | 2.6486 | . | . | no |
| H213 | H15 | 2.5719 | . | 1_545 | no |
| H215 | C218 | 2.9818 | . | 3_555 | no |
| H215 | H228' | 2.3782 | . | 3_555 | no |
| H216 | H218 | 2.4194 | . | . | no |
| H218 | C121 | 2.9515 | . | . | no |
| H218 | H216 | 2.4194 | . | . | no |
| H219 | O12 | 2.5749 | . | . | no |
| H222 | P2 | 2.9408 | . | . | no |
| H223 | H22 | 2.5997 | . | 4_555 | no |
| H224 | C22 | 3.0626 | . | 4_555 | no |
| H224 | C23 | 2.9846 | . | 4_555 | no |
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| H225 | C218 | 2.6281 | . | 1_455 | no |

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 H225    H127'        2.3338                    .     1_455                 no
 H228    O21          2.4780                    .       .                   no
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 H228    C124         2.8424                    .     3_455                 no

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#
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C128    H128    O12         0.9300     2.5300   2.985(2)     110.00     .   yes
C219    H219    O12         0.9100     2.5700   3.347(2)     143.00     .   yes
C228    H228    O21         1.0500     2.4800   2.967(2)     108.00     .   yes

#===END of Crystallographic Information File
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